Large-scale simulation of vortex liquid pinning in high-temperature superconductors

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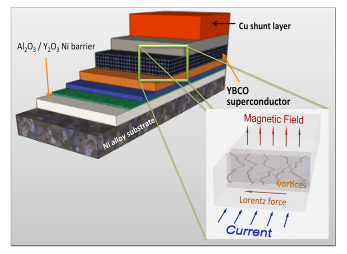
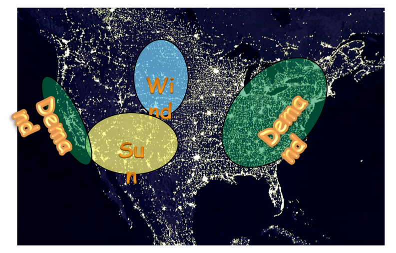
Motivation

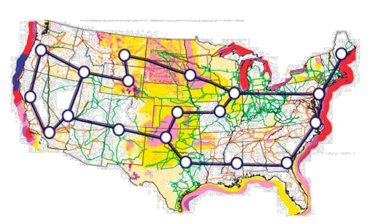
Applications

Superconducting cables and efficient energy delivery



Main obstacles to "superefficiency":
- Dissipative motion of disordered arrays of magnetic field vortices





Basic science

Understanding the behavior of complex driven systems

Vortex matter:
- Lattice (low T) → Melt → Liquid (high T)
- Control vortex liquid "viscosity" to minimize dissipation via inclusions

Vortex "avalanches"

Model

Time-dependent Ginzburg-Landau

$$\Gamma\left(\partial_t + i\frac{2e}{\hbar}\mu\right)\psi = a_0\epsilon(\mathbf{r})\psi - b|\psi|^2\psi + \frac{1}{4m}\left(\hbar\nabla + \frac{2e}{ic}\mathbf{A}\right)^2\psi + \zeta(\mathbf{r},t)$$

$$\underbrace{\frac{4pi}{c}\sigma\left(\frac{1}{c}\partial_t\mathbf{A} + \nabla\mu\right)}_{-\mathbf{J}_n} = \underbrace{-\frac{4pi}{c}\frac{e}{2m}\left[\psi^*\left(i\hbar\nabla + \frac{2e}{c}\mathbf{A}\right)\psi + c.c.\right]}_{-\mathbf{J}_s} - \nabla\times(\nabla\times\mathbf{A}) + \mathcal{I},$$

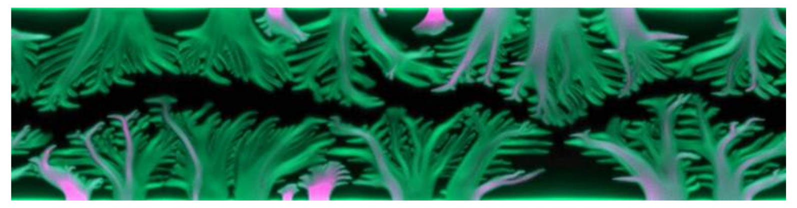
Coupled system for ψ and $\mathbf{A}$:

ψ	complex order parameter characterizing density of Cooper pairs
$\mathbf{A}$	vector potential for magnetic field
ζ and $\mathcal{I}$	fluctuations
Γ, a, b	phenomenological parameters from microscopic theory
$\epsilon(\mathbf{r}) = \frac{T_c(\mathbf{r})-T}{T} \to 0$	for $T \to T_c$ (critical temperature)

$$\mathbf{B} = \nabla\times\mathbf{A}, \quad \mathbf{E} = -\frac{1}{c}\partial_t\mathbf{A} - \nabla\mu$$

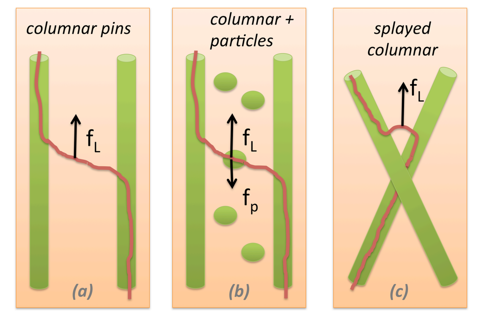
Extensions to TDGL

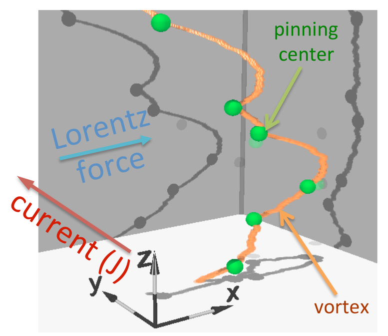
- *Coupling to temperature diffusion*
- *Effects of elastic strain*
- *Important both for applications and basic science*
- *Result in larger coupled systems*
- *Capture at the microlevel effects like penetration avalanches (macrosimulation below)*



Geometry

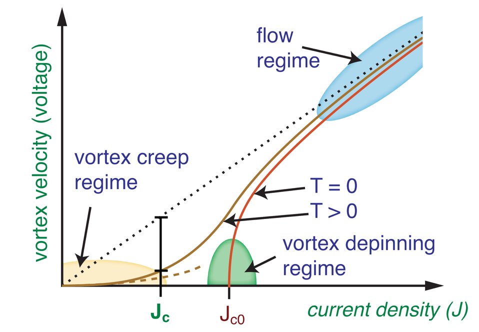
Magnetic vortices pinned by inclusions





Critical current enhanced by pinning

- *Critical current determined by long-time evolution of TDGL (to stationary flow)*
- *Dominated by rare events of vortex depinning and avalanches*
- *Frequency and duration of pinning/depinning depends on configurations of inclusions*
- *Suitable pinning configurations must be determined using geometry optimization*



Simulation

Long-time integration

- Need to obtain reliable statistics on J_s independent of transient, fluctuations
- Requires long-time integration ($\sim \Gamma/a_0$ millions of timesteps)
- Alleviated using implicit time-integration

$$\frac{\psi^{n+1}-\psi^n}{\Delta t} = \left(\frac{\epsilon}{u} - i\mu^{n+1}\right)\psi^{n+1} + \frac{1}{u}\Delta_{\mathbf{A}^{n+1}}\psi^{n+1} + F_i^{n+1} + F_e^n,$$

$$\frac{\mathbf{A}^{n+1}-\mathbf{A}^n}{\Delta t} = -\frac{c\kappa^2}{\sigma}\nabla\times(\nabla\times\mathbf{A}^{n+1}) + G_i^{n+1} + G_e^n,$$

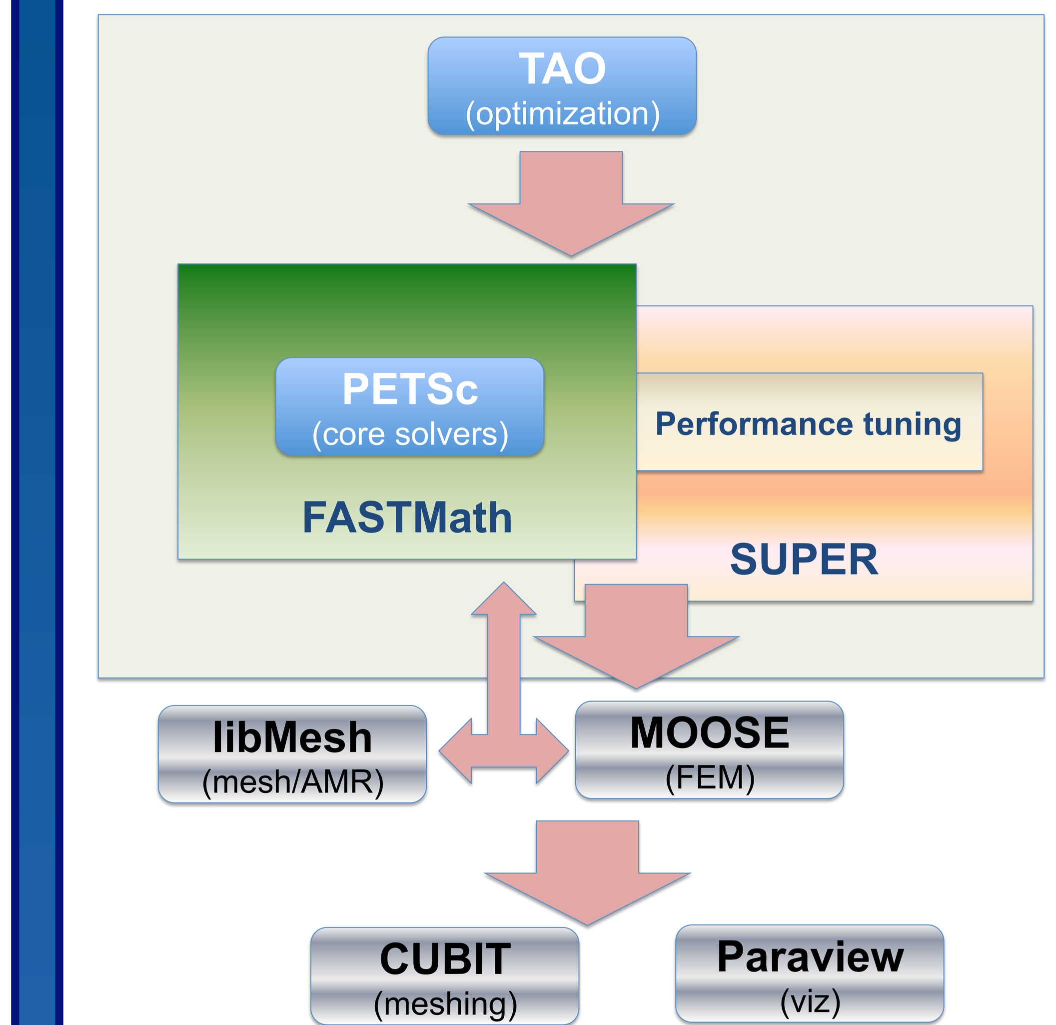
Parameters u and κ are related to Γ, a_0, b, ϵ as well as the fundamental coherence length ξ_0 and magnetic penetration length λ_0.

- $\psi^{n+1}, \mathbf{A}^{n+1}$ are the approximations at time t_{n+1} being determined from the approximations at t_n
- $\Delta_{\mathbf{A}} = (\nabla + i\mathbf{A})^2$ is the modified Laplace operator
- F_i^{n+1} and F_e^n are a splitting of the remaining nonlinear terms into implicit and explicit parts

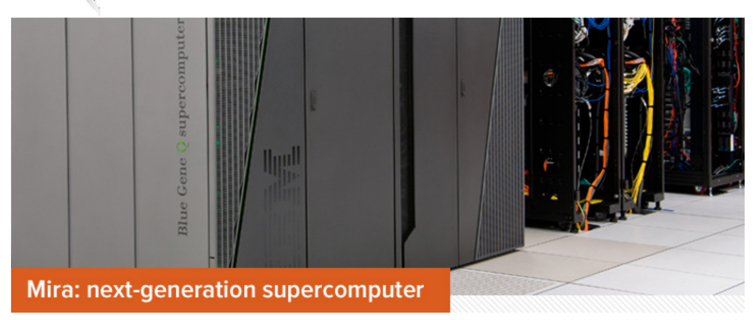
- Fully implicit methods correspond to $F_i = F,\ G_i = G,\ F_e = G_e = 0$ and generally enjoy the best stability properties.
- Linearly implicit methods (with $F_i = G_i = 0, \Delta_{\mathbf{A}^n} = \Delta$) have certain advantages
- Can be obtained as special cases of the general implicit method.

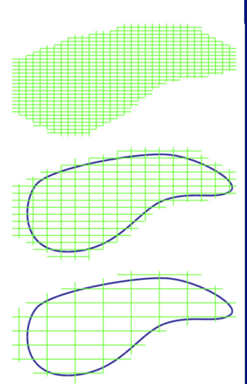
Software/algorithm stack

Leveraging power of SciDAC Institutes



Scalability





Convergence of time-step solve and scalability derives from properties of Jacobian:

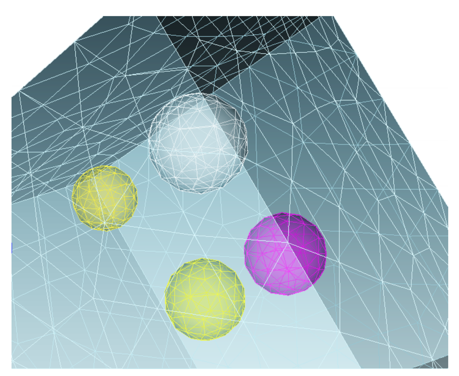
$$\mathcal{J} = \begin{pmatrix} M - \Delta t L_{\mathbf{A}} & \times \\ \times & \mathbf{M} + \Delta t\mathbf{K} \end{pmatrix}$$

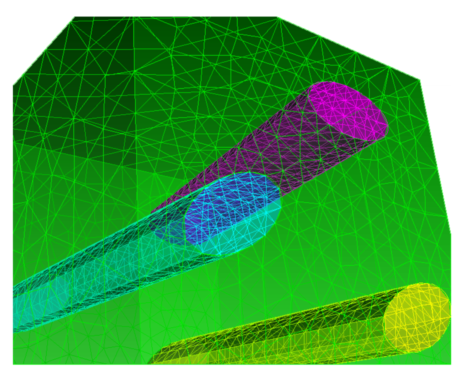
At $\mathcal{O}(1B)$ sizes this linear system must be solved iteratively, and Krylov subspace methods are the modern scalable approach of choice. Convergence of Krylov methods, however, crucially relies on the availability of an effective *preconditioner.*

- *physics-based* preconditioning,
  - combine effective preconditioners for (elliptic) diagonal blocks
- *multigrid*
  - AMG
  - GMG
  - appropriate treatment of the curl-curl operator
- *domain-decomposition* methods

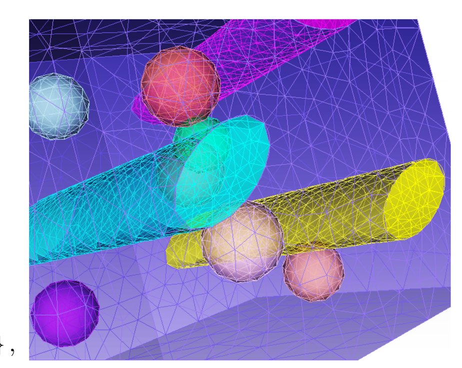
Sampling

Optimization of inclusion geometry





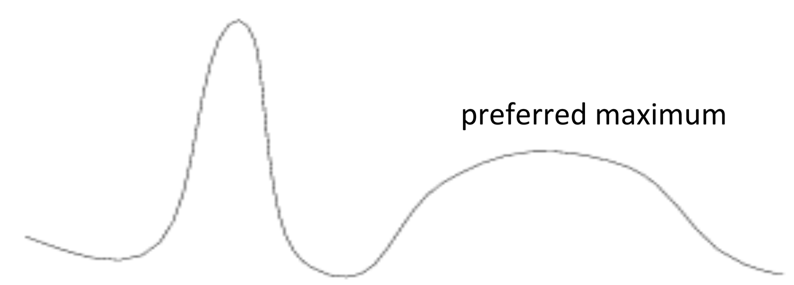
Determining optimal pinning landscape:
- Optimize critical current
- Minimize deviations from best case
- Min-max or min rms



$$\begin{aligned} \max_{\theta} \quad & J_c(\theta) \\ \text{such that} \quad & J_c(\theta) = \max_J \{J : V_\theta(J) \le \delta V_{ff}(J)\}, \\ & \theta \in \Theta. \end{aligned}$$

Objective function defined indirectly:
- Each value result of long-time simulation
- Must define optimal manufacturing parameters
- Without derivative information wrt $\theta = (d, e, g)$
- Eventually adjoint obtained via AD of simulation algorithms

Robust optimization

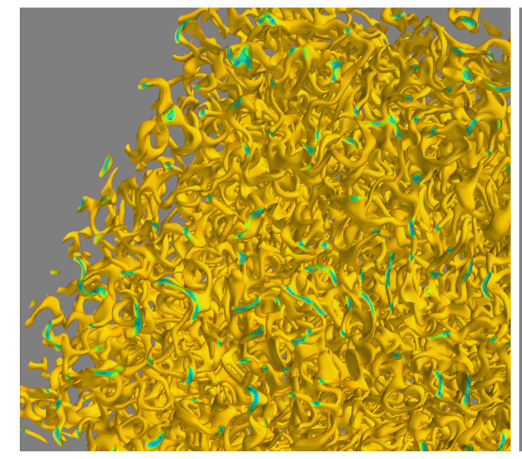


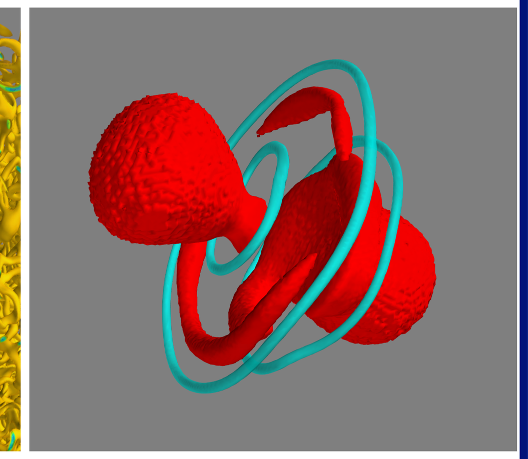
- Manufacturing might realize design close to target $\hat{\theta} = (\hat{d}, \hat{e}, \hat{g})$
- Such deviations must be tolerable
- Performance close to target

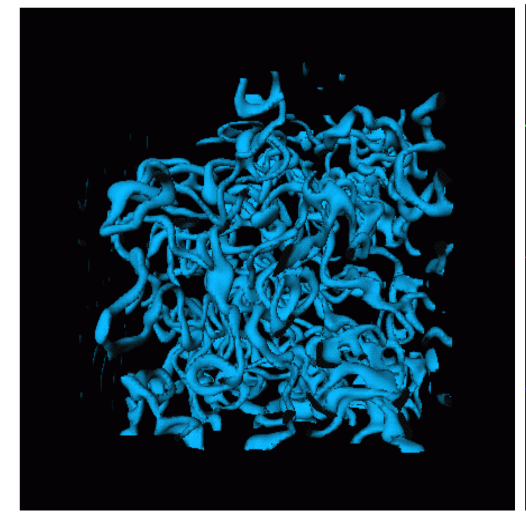
$$\begin{aligned} \max_{\theta} \quad & \max_{\omega} J_c(\omega) \\ \text{such that} \quad & J_c(\omega) = \max_J \{J : V_\omega(J) \le \delta V_{ff}(J)\}, \\ & \omega \in \Omega_\theta, \quad \theta \in \Theta, \end{aligned}$$

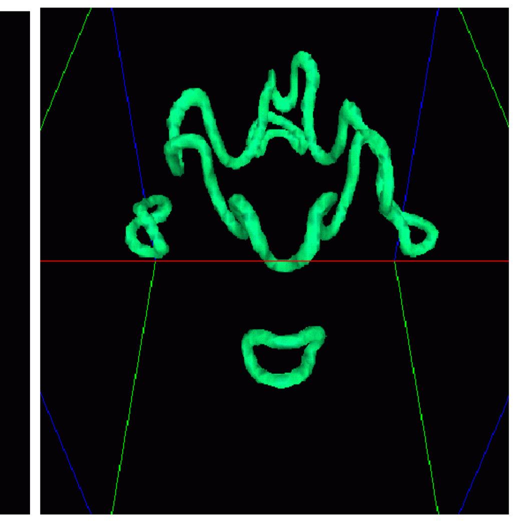
$$\Omega_\theta = \left\{(d,\ e,\ \hat{g}) : \hat{d} - \delta_d \le d \le \hat{d} + \delta_d; \hat{e} - \delta_e \le e \le \hat{e} + \delta_e, \right\}$$

Data Analysis & Visualization









Team

OSCon Organization Structure & Key Collaborations